Carbazole-2-carbonitrile, 5,6,7,8-tetrahydro-1-methyl-

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.70e-10 cm3/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 1.98e-01

Confidence level: 8.30e-01

Nearest Neighbors from the Training Set

Image not found
alpha-Phellandrene
Measured: 3.13e-10
Predicted: 2.83e-10

Image not found
alpha-Humalene
Measured: 2.90e-10
Predicted: 2.87e-10

Image not found
Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-
Measured: 4.80e-11
Predicted: 4.73e-11

Image not found
alpha-Terpinene
Measured: 3.63e-10
Predicted: 2.91e-10

Image not found
(3Z)-3-Hexenyl acetate
Measured: 7.80e-11
Predicted: 7.52e-11